



chain nodes :

1 2 3 10 11 12 13 14 15 22 23

ring nodes :

4 5 6 7 8 9 16 17 18 19 20 21

chain bonds :

1-2 1-5 2-3 2-22 10-22 10-23 10-11 11-12 12-13 12-14 13-15  
16-23

ring bonds :

4-5 4-9 5-6 6-7 7-8 8-9 16-17 16-21 17-18 18-19 19-20 20-21

exact/norm bonds :

1-2 1-5 2-3 10-11 11-12 12-13 12-14

exact bonds :

2-22 10-22 10-23 13-15 16-23

normalized bonds :

4-5 4-9 5-6 6-7 7-8 8-9 16-17 16-21 17-18 18-19 19-20 20-21

Match level :

1:CLASS 2:CLASS 3:CLASS 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom  
9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS  
16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS  
23:CLASS